1,2-Dibromoethylene

540)-49-8	DTXSID30602	4

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 8.55 days

Global applicability domain: Inside

Local applicability domain index: 4.38e-01

Confidence level: 7.09e-01

Nearest Neighbors from the Training Set

Image not found

1,2,4,5-Tetramethylbenzene

Measured: 88.3 **Predicted:** 5.46

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1,1-Dimethylcyclopentane

Measured: 880 Predicted: 10.9

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1,2,3,4-Tetramethylbenzene

Measured: 24.3 Predicted: 3.95

Image not found

2,2,3-Trimethylbutane

Measured: 61.9 Predicted: 10.7

Image not found

2,3,4-Trimethylpentane

Measured: 511 Predicted: 13.9